

Orthoformic acid, cyclic 2,2-dimethyltrimethylene ethyl ester
5783-79-9 | DTXSID20206542

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 4.06e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.55e-01

Confidence level: 8.32e-01

Nearest Neighbors from the Training Set

Image not found

1-Butoxy-2-propanol

Measured: 3.76e-11

Predicted: 3.73e-11

Image not found

2-(2-Butoxyethoxy)ethanol

Measured: 7.44e-11

Predicted: 5.15e-11

Image not found

Butane, 1,1'-
[methylenebis(oxy)]bis-

Measured: 3.39e-11

Predicted: 3.22e-11

Image not found

Diethylene glycol diethyl ether

Measured: 2.68e-11

Predicted: 2.50e-11